10520136b

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:21:22 ON 17 APR 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:21:26 ON 17 APR 2007

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 16 APR 2007 HIGHEST RN 930395-50-9
DICTIONARY FILE UPDATES: 16 APR 2007 HIGHEST RN 930395-50-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

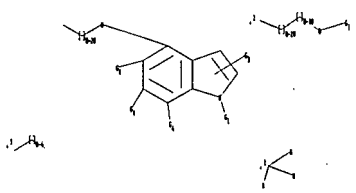
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

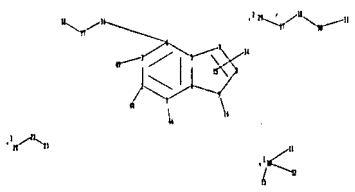
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\c10520136.str





chain nodes :

Karen Cheng

10520136b

10 11 12 13 16 17 18 21 22 23 29 30 31 34 36 37 38 43 44 46
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-46 2-44 3-43 4-36 9-16 10-11 10-12 10-13 17-18 17-29 18-30 21-22
22-23 30-31 36-37 37-38
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-46 2-44 3-43 4-36 5-7 6-9 7-8 8-9 9-16 18-30 30-31 36-37
exact bonds :
10-11 10-12 10-13 17-18 17-29 21-22 22-23 37-38
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,[*1]

G3:H,[*2]

G4:H,[*3]

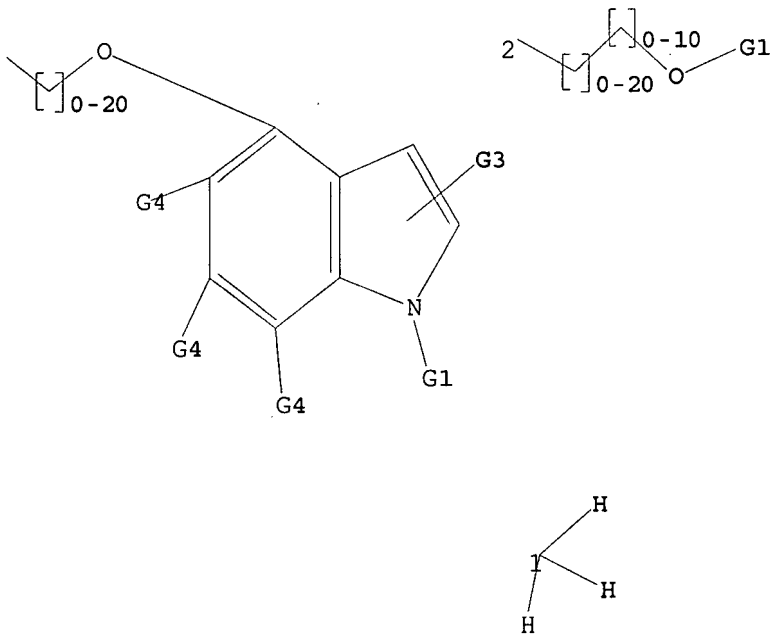
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS 22:CLASS
23:CLASS 29:CLASS 30:CLASS 31:CLASS 34:CLASS 35:Atom 36:CLASS 37:CLASS
38:CLASS 43:CLASS 44:CLASS 46:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR

Karen Cheng

10520136b



G1 H, [@1]

G2

G3 H, [@2]

G4 H, [@3]

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 full
FULL SEARCH INITIATED 15:22:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   116074 TO ITERATE

100.0% PROCESSED   116074 ITERATIONS                          3887 ANSWERS
SEARCH TIME: 00.00.01

L2          3887 SEA SSS FUL L1

=> s l2 and 1/N
       5406524 1/N
L3          409 L2 AND 1/N

=> s l3 and 2/O
       6107828 2/O
L4           89 L3 AND 2/O

=>
Uploading C:\Program Files\Stnexp\Queries\d10520136.str
```

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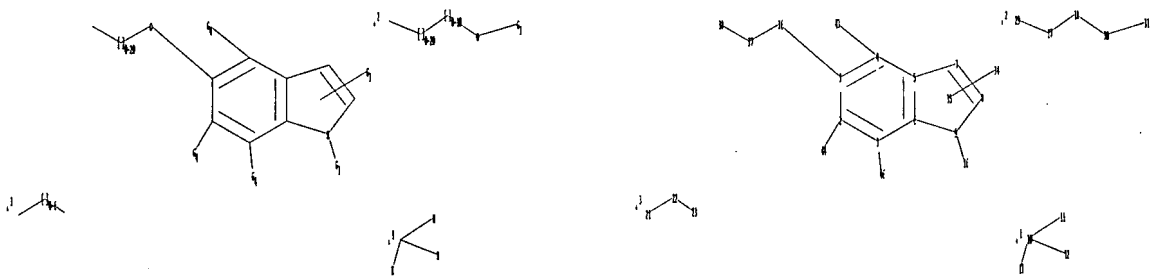
10520136b



chain nodes :
10 11 12 13 16 17 18 21 22 23 29 30 31 34 36 37 38 43 44 46
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-46 2-44 3-36 4-43 9-16 10-11 10-12 10-13 17-18 17-29 18-30 21-22
22-23 30-31 36-37 37-38
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-46 2-44 3-36 4-43 5-7 6-9 7-8 8-9 9-16 18-30 30-31 36-37
exact bonds :
10-11 10-12 10-13 17-18 17-29 21-22 22-23 37-38
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,[*1]

G3:H,[*2]

G4:H,[*3]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS 22:CLASS
23:CLASS 29:CLASS 30:CLASS 31:CLASS 34:CLASS 35:Atom 36:CLASS 37:CLASS
38:CLASS 43:CLASS 44:CLASS 46:CLASS

L5 STRUCTURE UPLOADED

Karen Cheng

10520136b

```
=> d
L5 HAS NO ANSWERS
L5              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l5 full
FULL SEARCH INITIATED 15:22:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   264647 TO ITERATE

100.0% PROCESSED   264647 ITERATIONS                          13522 ANSWERS
SEARCH TIME: 00.00.02

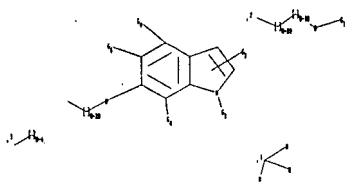
L6         13522 SEA SSS FUL L5

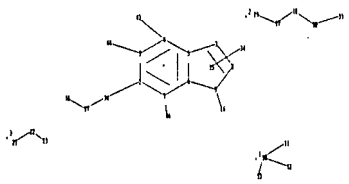
=> s l5 and 1/N
COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
The query entered contains both search terms created by
structure-building or screen commands and text search terms.  L#s
created via the STRUCTURE or SCREEN commands must be searched in the
structures files separately from text terms or profiles.  The L#
answer sets from structure searches can be used in crossover searches
and can be combined with text terms.

=> s l6 and 1/N
       5406524 1/N
L7        1940 L6 AND 1/N

=> s l7 and 2/O
       6107828 2/O
L8         325 L7 AND 2/O

=>
Uploading C:\Program Files\Stnexp\Queries\e10520136.str
```





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10520136b

chain nodes :
10 11 12 13 16 17 18 21 22 23 29 30 31 34 36 37 38 43 44 46
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-46 2-36 3-44 4-43 9-16 10-11 10-12 10-13 17-18 17-29 18-30 21-22
22-23 30-31 36-37 37-38
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-46 2-36 3-44 4-43 5-7 6-9 7-8 8-9 9-16 18-30 30-31 36-37
exact bonds :
10-11 10-12 10-13 17-18 17-29 21-22 22-23 37-38
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,[*1]

G3:H,[*2]

G4:H,[*3]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS 22:CLASS
23:CLASS 29:CLASS 30:CLASS 31:CLASS 34:CLASS 35:Atom 36:CLASS 37:CLASS
38:CLASS 43:CLASS 44:CLASS 46:CLASS

L9 STRUCTURE UPLOADED

=> d
L9 HAS NO ANSWERS
L9 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l9 full
FULL SEARCH INITIATED 15:23:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 260147 TO ITERATE

100.0% PROCESSED 260147 ITERATIONS 3038 ANSWERS
SEARCH TIME: 00.00.01

L10 3038 SEA SSS FUL L9

=> s l10 and 1/N
5406524 1/N
L11 362 L10 AND 1/N

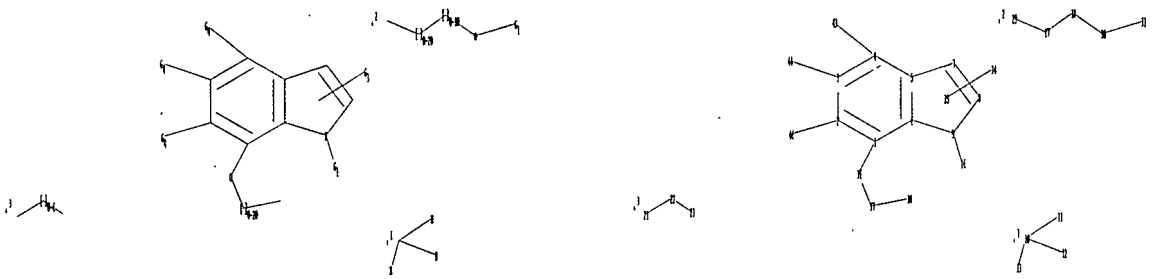
=> s l11 and 2/O
6107828 2/O

Karen Cheng

10520136b

L12 61 L11 AND 2/O

=>
Uploading C:\Program Files\Stnexp\Queries\f10520136.str



chain nodes :
10 11 12 13 16 17 18 21 22 23 29 30 31 34 36 37 38 43 44 46
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-36 2-46 3-44 4-43 9-16 10-11 10-12 10-13 17-18 17-29 18-30 21-22
22-23 30-31 36-37 37-38
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-36 2-46 3-44 4-43 5-7 6-9 7-8 8-9 9-16 18-30 30-31 36-37
exact bonds :
10-11 10-12 10-13 17-18 17-29 21-22 22-23 37-38
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,[*1]

G3:H,[*2]

G4:H,[*3]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS 22:CLASS
23:CLASS 29:CLASS 30:CLASS 31:CLASS 34:CLASS 35:Atom 36:CLASS 37:CLASS
38:CLASS 43:CLASS 44:CLASS 46:CLASS

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L13 STRUCTURE UPLOADED

=> d
L13 HAS NO ANSWERS
L13 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l13 full
FULL SEARCH INITIATED 15:24:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 95445 TO ITERATE

100.0% PROCESSED 95445 ITERATIONS 1358 ANSWERS
SEARCH TIME: 00.00.01

L14 1358 SEA SSS FUL L13

=> s l14 and 1/N
5406524 1/N
L15 198 L14 AND 1/N

=> s l15 and 2/O
6107828 2/O
L16 48 L15 AND 2/O

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	728.45	728.66

FILE 'CAPLUS' ENTERED AT 15:24:39 ON 17 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 17 Apr 2007 VOL 146 ISS 17
FILE LAST UPDATED: 15 Apr 2007 (20070415/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> d his

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(FILE 'HOME' ENTERED AT 15:21:22 ON 17 APR 2007)

FILE 'REGISTRY' ENTERED AT 15:21:26 ON 17 APR 2007

```
L1              STRUCTURE UPLOADED
L2          3887 S L1 FULL
L3           409 S L2 AND 1/N
L4            89 S L3 AND 2/O
L5              STRUCTURE UPLOADED
L6         13522 S L5 FULL
L7          1940 S L6 AND 1/N
L8           325 S L7 AND 2/O
L9              STRUCTURE UPLOADED
L10         3038 S L9 FULL
L11          362 S L10 AND 1/N
L12           61 S L11 AND 2/O
L13             STRUCTURE UPLOADED
L14         1358 S L13 FULL
L15          198 S L14 AND 1/N
L16           48 S L15 AND 2/O
```

FILE 'CAPLUS' ENTERED AT 15:24:39 ON 17 APR 2007

```
=> s (l4 or l8 or l12 or l16)
           208 L4
           828 L8
           134 L12
            69 L16
L17       1106 (L4 OR L8 OR L12 OR L16)

=> dup rem l17
PROCESSING IS APPROXIMATELY  95% COMPLETE FOR L17
PROCESSING COMPLETED FOR L17
L18        1105 DUP REM L17 (1 DUPLICATE REMOVED)
             ANSWERS '1-1105' FROM FILE CAPLUS

=> fil stng
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                               0.94     729.60

FILE 'STNGUIDE' ENTERED AT 15:25:46 ON 17 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Apr 13, 2007 (20070413/UP).

=> fil reg
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                               0.48     730.08

FILE 'REGISTRY' ENTERED AT 15:30:17 ON 17 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.
```

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STRUCTURE FILE UPDATES: 16 APR 2007 HIGHEST RN 930395-50-9
DICTIONARY FILE UPDATES: 16 APR 2007 HIGHEST RN 930395-50-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

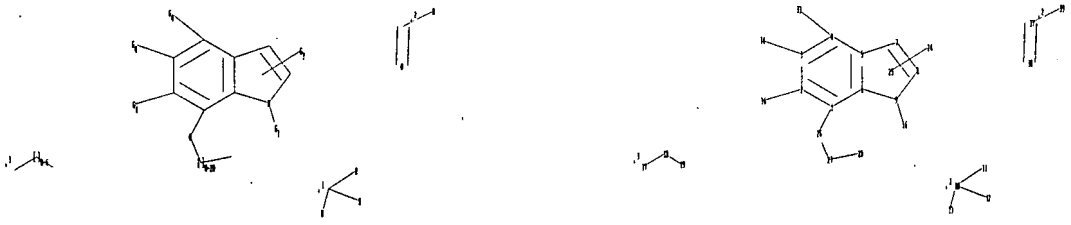
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>
Uploading C:\Program Files\Stnexp\Queries\ff10520136.str



chain nodes :
10 11 12 13 16 17 18 19 24 26 27 28 33 34 36 37 38 39
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-26 2-36 3-34 4-33 9-16 10-11 10-12 10-13 17-18 18-19 26-27 27-28 37-38 37-39

Karen Cheng

10520136b

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-26 2-36 3-34 4-33 5-7 6-9 7-8 8-9 9-16 26-27 37-38
exact bonds :
10-11 10-12 10-13 17-18 18-19 27-28 37-39
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,[*1]

G3:H,[*2]

G4:H,[*3]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 24:CLASS
25:Atom 26:CLASS 27:CLASS 28:CLASS 33:CLASS 34:CLASS 36:CLASS 37:CLASS
38:CLASS 39:CLASS

L19 STRUCTURE UPLOADED

=> que L19

L20 QUE L19

=> d
L20 HAS NO ANSWERS
L19 STR

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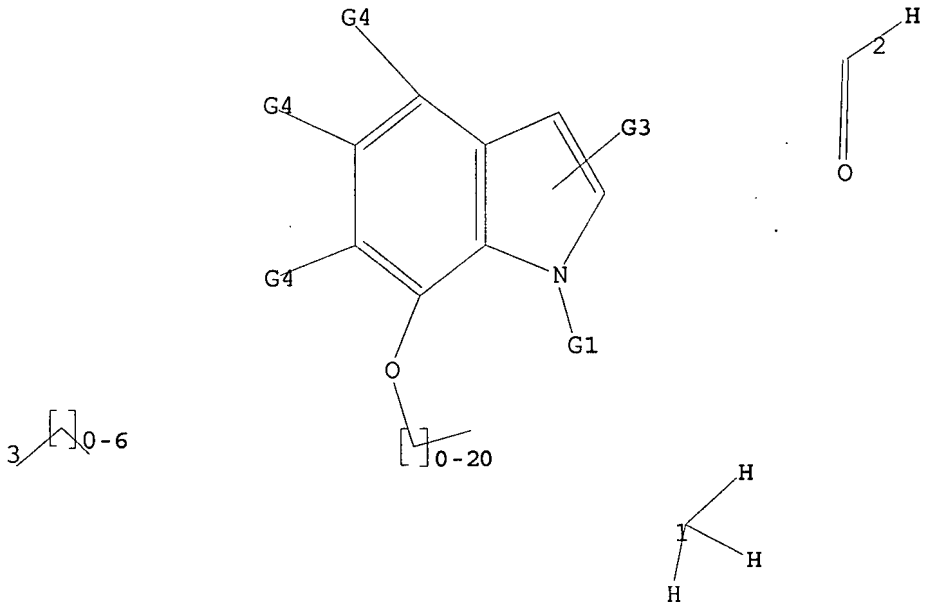
10520136b



G1 H, [@1]

G2

G3 H, [@2]

G4 H, [@3]

Structure attributes must be viewed using STN Express query preparation.
L20 QUE ABB=ON PLU=ON L19

not full search

=> s l20
SAMPLE SEARCH INITIATED 15:30:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 4795 TO ITERATE

41.7% PROCESSED 2000 ITERATIONS 35 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 91748 TO 100052
PROJECTED ANSWERS: 1129 TO 2227

L21 35 SEA SSS SAM L19

=> s l16 not l21
L22 47 L16 NOT L21

=>
Uploading C:\Program Files\Stnexp\Queries\ee10520136.str

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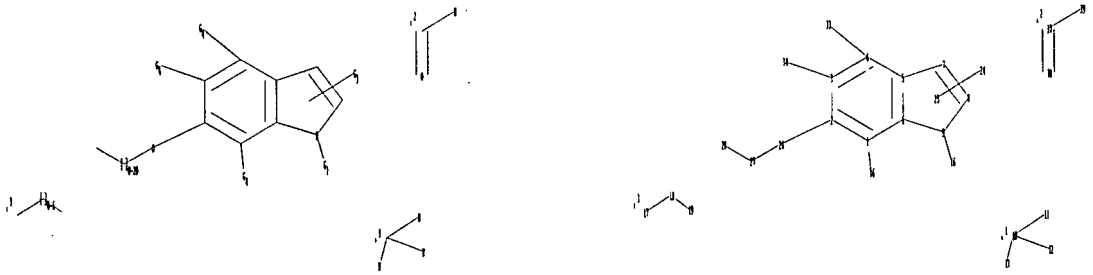
10520136b



chain nodes :
10 11 12 13 16 17 18 19 24 26 27 28 33 34 36 37 38 39
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-36 2-26 3-34 4-33 9-16 10-11 10-12 10-13 17-18 18-19 26-27 27-28
37-38 37-39
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-36 2-26 3-34 4-33 5-7 6-9 7-8 8-9 9-16 26-27 37-38
exact bonds :
10-11 10-12 10-13 17-18 18-19 27-28 37-39
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,[*1]

G3:H,[*2]

G4:H,[*3]

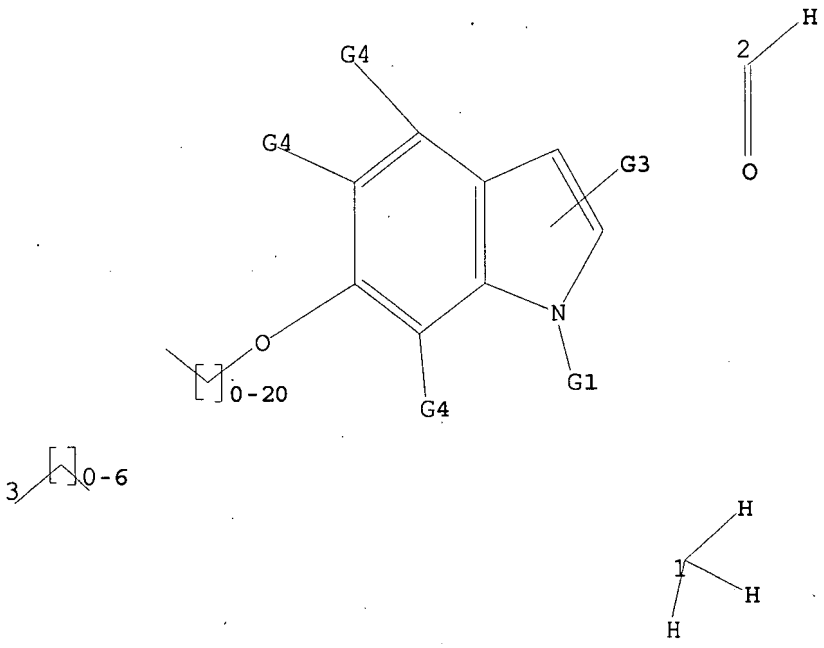
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 24:CLASS
25:Atom 26:CLASS 27:CLASS 28:CLASS 33:CLASS 34:CLASS 36:CLASS 37:CLASS
38:CLASS 39:CLASS

L23 STRUCTURE UPLOADED

Karen Cheng

10520136b

=> d
L23 HAS NO ANSWERS
L23 STR



G1 H, [@1]

G2

G3 H, [@2]

G4 H, [@3]

Structure attributes must be viewed using STN Express query preparation.

=> s l23
SAMPLE SEARCH INITIATED 15:33:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 12987 TO ITERATE

15.4% PROCESSED 2000 ITERATIONS 18 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 252913 TO 266567
PROJECTED ANSWERS: 1689 TO 2985

L24 18 SEA SSS SAM L23

=> s l23 full
FULL SEARCH INITIATED 15:33:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 260147 TO ITERATE

100.0% PROCESSED 260147 ITERATIONS 2583 ANSWERS
SEARCH TIME: 00.00.02

Karen Cheng

10520136b

```
L25         2583 SEA SSS FUL L23

=> s l12 not l25
L26            1 L12 NOT L25
=> d his

     (FILE 'HOME' ENTERED AT 15:21:22 ON 17 APR 2007)

     FILE 'REGISTRY' ENTERED AT 15:21:26 ON 17 APR 2007
L1               STRUCTURE UPLOADED
L2          3887 S L1 FULL
L3           409 S L2 AND 1/N
L4            89 S L3 AND 2/O
L5               STRUCTURE UPLOADED
L6         13522 S L5 FULL
L7          1940 S L6 AND 1/N
L8           325 S L7 AND 2/O
L9               STRUCTURE UPLOADED
L10         3038 S L9 FULL
L11          362 S L10 AND 1/N
L12           61 S L11 AND 2/O
L13              STRUCTURE UPLOADED
L14         1358 S L13 FULL
L15          198 S L14 AND 1/N
L16           48 S L15 AND 2/O

     FILE 'CAPLUS' ENTERED AT 15:24:39 ON 17 APR 2007
L17         1106 S (L4 OR L8 OR L12 OR L16)
L18         1105 DUP REM L17 (1 DUPLICATE REMOVED)

     FILE 'STNGUIDE' ENTERED AT 15:25:46 ON 17 APR 2007

     FILE 'REGISTRY' ENTERED AT 15:30:17 ON 17 APR 2007
L19              STRUCTURE UPLOADED
L20              QUE L19
L21            35 S L20
L22            47 S L16 NOT L21
L23              STRUCTURE UPLOADED
L24            18 S L23
L25          2583 S L23 FULL
L26             1 S L12 NOT L25

=> s l20 full
FULL SEARCH INITIATED 15:34:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    95445 TO ITERATE

100.0% PROCESSED    95445 ITERATIONS                          1288 ANSWERS
SEARCH TIME: 00.00.01

L27          1288 SEA SSS FUL L19

=> s l16 not l27
L28             1 L16 NOT L27

=>
Uploading C:\Program Files\Stnexp\Queries\dd10520136.str
```

1105 hits

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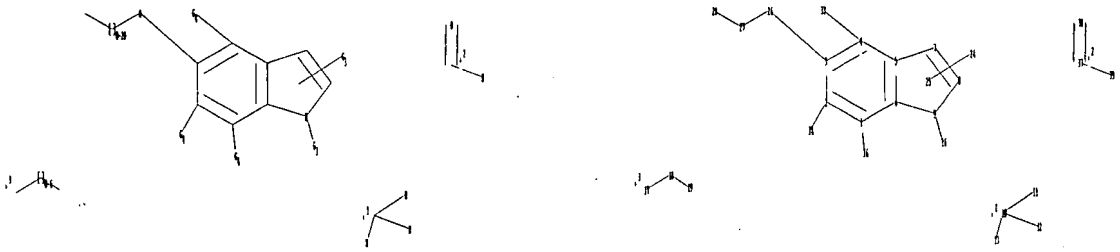
10520136b



chain nodes :
10 11 12 13 16 17 18 19 24 26 27 28 33 34 36 37 38 39
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-36 2-34 3-26 4-33 9-16 10-11 10-12 10-13 17-18 18-19 26-27 27-28
37-38 37-39
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-36 2-34 3-26 4-33 5-7 6-9 7-8 8-9 9-16 26-27 37-38
exact bonds :
10-11 10-12 10-13 17-18 18-19 27-28 37-39
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,[*1]

G3:H,[*2]

G4:H,[*3]

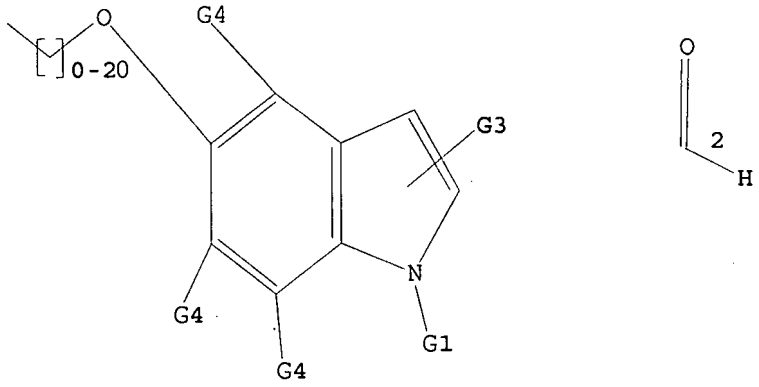
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 24:CLASS
25:Atom 26:CLASS 27:CLASS 28:CLASS 33:CLASS 34:CLASS 36:CLASS 37:CLASS
38:CLASS 39:CLASS

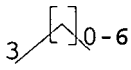
L29 STRUCTURE UPLOADED

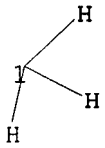
Karen Cheng

10520136b

=> d
L29 HAS NO ANSWERS
L29 STR







G1 H, [@1]

G2

G3 H, [@2]

G4 H, [@3]

Structure attributes must be viewed using STN Express query preparation.

=> s l29 full
FULL SEARCH INITIATED 15:36:55 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 264647 TO ITERATE

100.0% PROCESSED 264647 ITERATIONS 11812 ANSWERS
SEARCH TIME: 00.00.02

L30 11812 SEA SSS FUL L29

=> s l8 not l30
L31 13 L8 NOT L30

=>
Uploading C:\Program Files\Stnexp\Queries\cc10520136.str

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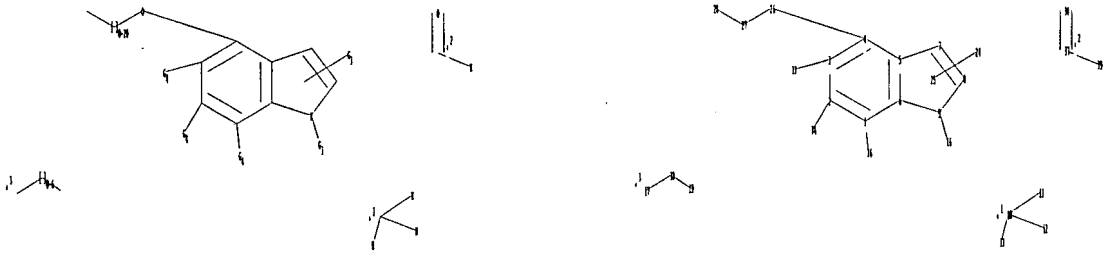
10520136b



chain nodes :
10 11 12 13 16 17 18 19 24 26 27 28 33 34 36 37 38 39
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-36 2-34 3-33 4-26 9-16 10-11 10-12 10-13 17-18 18-19 26-27 27-28
37-38 37-39
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-36 2-34 3-33 4-26 5-7 6-9 7-8 8-9 9-16 26-27 37-38
exact bonds :
10-11 10-12 10-13 17-18 18-19 27-28 37-39
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,[*1]

G3:H,[*2]

G4:H,[*3]

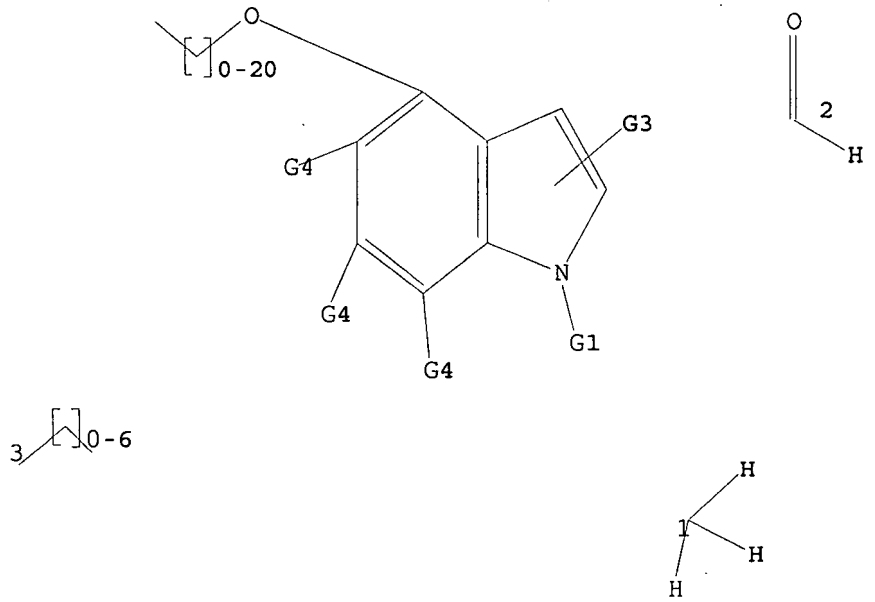
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 24:CLASS
25:Atom 26:CLASS 27:CLASS 28:CLASS 33:CLASS 34:CLASS 36:CLASS 37:CLASS
38:CLASS 39:CLASS

L32 STRUCTURE UPLOADED

Karen Cheng

10520136b

=> d
L32 HAS NO ANSWERS
L32 STR



G1 H, [@1]

G2

G3 H, [@2]

G4 H, [@3]

Structure attributes must be viewed using STN Express query preparation.

=> s l32 full
FULL SEARCH INITIATED 15:38:19 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 116074 TO ITERATE

100.0% PROCESSED 116074 ITERATIONS 3745 ANSWERS
SEARCH TIME: 00.00.01

L33 3745 SEA SSS FUL L32

=> s l4 not l33
L34 3 L4 NOT L33

=> d his

(FILE 'HOME' ENTERED AT 15:21:22 ON 17 APR 2007)

FILE 'REGISTRY' ENTERED AT 15:21:26 ON 17 APR 2007
L1 STRUCTURE UPLOADED
L2 3887 S L1 FULL
L3 409 S L2 AND 1/N
L4 89 S L3 AND 2/O
L5 STRUCTURE UPLOADED
L6 13522 S L5 FULL

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10520136b

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L7          1940 S L6 AND 1/N
L8           325 S L7 AND 2/O
L9               STRUCTURE UPLOADED
L10         3038 S L9 FULL
L11          362 S L10 AND 1/N
L12           61 S L11 AND 2/O
L13              STRUCTURE UPLOADED
L14         1358 S L13 FULL
L15          198 S L14 AND 1/N
L16           48 S L15 AND 2/O

     FILE 'CAPLUS' ENTERED AT 15:24:39 ON 17 APR 2007
L17         1106 S (L4 OR L8 OR L12 OR L16)
L18         1105 DUP REM L17 (1 DUPLICATE REMOVED)

     FILE 'STNGUIDE' ENTERED AT 15:25:46 ON 17 APR 2007

     FILE 'REGISTRY' ENTERED AT 15:30:17 ON 17 APR 2007
L19              STRUCTURE UPLOADED
L20              QUE L19
L21            35 S L20
L22            47 S L16 NOT L21
L23              STRUCTURE UPLOADED
L24            18 S L23
L25          2583 S L23 FULL
L26             1 S L12 NOT L25
L27          1288 S L20 FULL
L28             1 S L16 NOT L27
L29              STRUCTURE UPLOADED
L30         11812 S L29 FULL
L31            13 S L8 NOT L30
L32              STRUCTURE UPLOADED
L33          3745 S L32 FULL
L34             3 S L4 NOT L33

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             693.35    1423.43

FILE 'CAPLUS' ENTERED AT 15:39:28 ON 17 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 17 Apr 2007  VOL 146 ISS 17
FILE LAST UPDATED: 15 Apr 2007  (20070415/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
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Karen Cheng

10520136b

They are available for your review at:

http://www.cas.org/infopolicy.html

```
=> s (l26 or l28 or l31 or l34)
             1 L26
             2 L28
            12 L31
             2 L34
L35         16 (L26 OR L28 OR L31 OR L34)

=> d ibib abs hitstr tot
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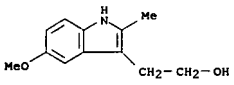
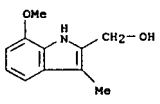
Karen Cheng

L35 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1187102 CAPLUS
DOCUMENT NUMBER: 144:45008
TITLE: Indolyl esters and amides related to indomethacin are selective COX-2 inhibitors
AUTHOR(S): Kalgutkar, Amit S.; Crews, Brenda C.; Saleh, Sam; Prudhomme, Daniel; Marnett, Lawrence J.
CORPORATE SOURCE: A.B. Hancock, Jr., Memorial Laboratory for Cancer Research, Departments of Biochemistry and Chemistry, Vanderbilt Institute of Chemical Biology, Center in Molecular Toxicology, Vanderbilt University School of Medicine, Nashville, TN, 37232-0146, USA
SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(24), 6810-6822
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:45008
AB Previous studies from our laboratory have revealed that esterification/amidation of the carboxylic acid moiety in the nonsteroidal anti-inflammatory drug, indomethacin, generates potent and selective COX-2 inhibitors. In the present study, a series of reverse ester/amide derivs. were synthesized and evaluated as selective COX-2 inhibitors. Most of the reverse esters/amides displayed time-dependent COX-2 inhibition with IC50 values in the low nanomolar range. Replacement of the 4-chlorobenzoyl group on the indole nitrogen with a 4-bromobenzyl moiety resulted in compds. that retained selective COX-2 inhibitory potency. In addition to inhibiting COX-2 activity in vitro, the reverse esters/amides also inhibited COX-2 activity in the mouse macrophage-like cell line, RAW264.7. Overall, this strategy broadens the scope of our previous methodol. of neutralizing the carboxylic acid group in NSAIDs as a means of generating COX-2-selective inhibitors and is potentially applicable to other NSAIDs.
IT 26766-01-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(indolyl esters and amides related to indomethacin as selective COX-2 inhibitors)
RN 26766-01-8 CAPLUS
CN 1H-Indole-3-ethanol, 5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:648700 CAPLUS
DOCUMENT NUMBER: 140:253397
TITLE: The chemistry of indoles. 121. The first preparation of the unstable 1-hydroxy-2,3-dimethylindole, and structural determination of its air-oxidized product, 3-hydroxy-2,3-dimethyl-3H-indole N-oxide
AUTHOR(S): Yamada, Fumio; Kawanishi, Atsuko; Tomita, Akiko; Somei, Masanori
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Kanazawa University, Kanazawa, 920-0934, Japan
SOURCE: ARKIVOC (Gainesville, FL, United States) (2003), (8), 102-111
CODEN: AGFUAR
URL: http://www.arkat-usa.org/ark/journal/2003/Fukumoto/KF-770H/770H.pdf
PUBLISHER: Arkat USA Inc.
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:253397
AB 1-Hydroxy-2,3-dimethylindole (I) has been prepared for the first time. Under atmospheric oxygen, I was converted rapidly into 3-hydroxy-2,3-dimethyl-3H-indole N-oxide (II). The structure of II was deduced, based on its products obtained by the reaction with Ac2O in pyridine and confirmed by x-ray single crystallog. anal.
IT 30464-84-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and air oxidation of hydroxydimethylindole and crystal structure of hydroxydimethylindole oxide)
RN 30464-84-7 CAPLUS
CN Indole-2-methanol, 7-methoxy-3-methyl- (8CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L35 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:816638 CAPLUS
DOCUMENT NUMBER: 135:357839
TITLE: Preparation of bicyclic compounds such as benzofuran, indole, benzothiofuran, and indene derivatives of phenylethanolamine as β adrenoreceptor agonists
INVENTOR(S): Ikuta, Shunichi; Miyoshi, Shiro; Ogawa, Kohei
PATENT ASSIGNEE(S): Asahi Kasei Kabushiki Kaisha, Japan
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001083451	A1	20011108	WO 2001-JP3575	20010425
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 200152574	A	20011112	AU 2001-52574	20010425
CA 2407538	A1	20021025	CA 2001-2407538	20010425
CA 2407538	C	20070109		
EP 1277736	A1	20030122	EP 2001-925911	20010425
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003191174	A1	20031009	US 2002-258817	20021028
US 6861444	B2	20050301		
US 2004127546	A1	20040701	US 2004-761265	20040122
US 7049445	B2	20060523		

PRIORITY APPLN. INFO.: JP 2000-130414 A 20000428
WO 2001-JP3575 W 20010425
US 2002-258817 A3 20021028

OTHER SOURCE(S): MARPAT 135:357839
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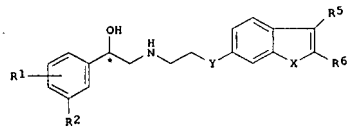


I

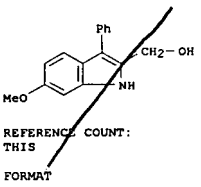
L35 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB Compds. of the general formula (I) or salts thereof [wherein R1 is hydrogen, hydroxy, or halo; R2 is NHSO2R3, SO2NR4R4' (wherein R3 is C1-6 alkyl, benzyl, Ph, or NR4R4'; R4, R4' = H or C1-6 alkyl); R5 and R6 are each independently hydrogen, C1-6 alkyl, optionally substituted Ph, or benzyl; X is NH, sulfur, oxygen, or methylene; Y is oxygen, NR7, sulfur, methylene, or a bond (wherein R7 is H, C1-6 alkyl, or C1-6 acyl); and * represents an asym. carbon atom.] are prepared These compds. exhibit a potent and selective stimulating activity for human β3 adrenoreceptor with very little effect on increasing heart beat of guinea pigs and are useful as preventive and therapeutic drugs for diabetes, obesity, hyperlipidemia, digestive system diseases, depression, and urinary disorders. Thus, N-(3-bromoacetylphenyl)methanesulfonamide, 2-(2,3-dimethyl-1H-indol-6-yloxy)ethylamine, and Et3N were added to DMF, stirred at room temperature for 1 h, treated with a solution of NaBH4 in ethanol, and stirred at room temperature for 5 h to give, after purification on a reversed phase column, N-[3-[2-[[2-(2,3-dimethyl-1H-indol-6-yloxy)ethyl]amino]-1-hydroxyethyl]phenyl]methanesulfonamide trifluoroacetate salt (II). II was as potent as isoproterenol for stimulating the production of cAMP in CHO cell line expressing human β3 adrenoreceptor (Ed50 of 8.7 nM).

IT 372094-03-6P, 2-Hydroxymethyl-6-methoxy-3-phenyl-1H-indole
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bicyclic compds. such as benzofuran, indole, benzothiofuran, and indoline derivs. of phenylethanolamine as β adrenoreceptor agonists and preventive and therapeutic drugs)

RN 372094-03-6 CAPLUS

CN 1H-Indole-2-methanol, 6-methoxy-3-phenyl- (9CI) (CA INDEX NAME)



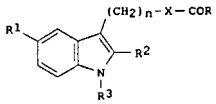
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:167797 CAPLUS
DOCUMENT NUMBER: 134:207711
TITLE: Preparation of selective COX-2 inhibitory novel esters from indolealkanols and novel amides from indolealkylamines
INVENTOR(S): Kalgutkar, Amit S.; Marnett, Lawrence J.
PATENT ASSIGNEE(S): Vanderbilt University, USA
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001015686	A1	20010308	WO 2000-US23153	20000823
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6306890	B1	20011023	US 1999-385748	19990830
CA 2382296	A1	20010308	CA 2000-2382296	20000823
EP 1225882	A1	20020731	EP 2000-957717	20000823
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003508433	T	20030304	JP 2001-519900	20000823
AU 772334	B2	20040422	AU 2000-69297	20000823
PRIORITY APPLN. INFO.:			US 1999-385748 A	19990830
			WO 2000-US23153 W	20000823

OTHER SOURCE(S): MARPAT 134:207711
GI



I

AB Indolealkanol esters and indolealkylamides of the compound of the formula [I; R = (un)branched C1-6 alkyl, C4-8 cycloalkyl, (un)branched C1-6 hydroxyalkyl, hydroxy-substituted C4-8 aryl, primary, secondary or

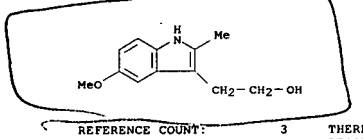
L35 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

tertiary (un)branched C1-6 alkylamino, primary, secondary or tertiary C4-8 arylamino, (un)branched C1-6 alkylcarboxylic acid, (un)branched C1-6 alkyl ester, C4-8 aryl, C4-8 arylcarboxylic acid, etc.; R1 = (un)branched C1-6 alkyl, C4-8 cycloalkyl, C4-8 aryl, C4-8 aryl-substituted C1-6 alkyl, (un)branched C1-6 alkoxy, C4-8 aryloxy, or halo-substituted versions thereof or R1 is halo where halo is chloro, fluoro, bromo, or iodo; R2 = hydrogen, (un)branched C1-6 alkyl; R3 = C1-6 alkyl, C4-8 aroyl, C4-8 aryl, C4-8 heterocyclic alkyl or aryl with O, N or S in the ring, C4-8 aryl-substituted C1-6 alkyl, alkyl-substituted or aryl-substituted C4-8 heterocyclic alkyl or aryl with O, N or S in the ring, alkyl-substituted C4-8 aroyl, or alkyl-substituted C4-8 aryl, or halo-substituted versions thereof or R1 is halo where halo is chloro, bromo, or iodo; n = 1,2, 3, or 4; and X = O, NH, or N-R4, where R4 = (un)branched alkyl] are prepd. These compds. are selective cyclooxygenase-2 (COX-2) inhibitors and useful as analgesic, antiinflammatory, or antipyretic agents. Thus, NaH was added to a soln. of 5-methoxy-2-methylindole-3-Et p-methoxybenzoate in DMF at 0° and stirred at 0° for 20 min and treated with 4-chlorobenzoyl chloride and then stirred overnight to give N-(p-chlorobenzoyl)-5-methoxy-2-methylindole-3-Et p-methoxybenzoate (II). II showed IC50 of 0.04 and >66 μM against COX-2 and COX-1, resp., with >1,466-times selectivity for COX-2.

IT 26766-01-8P, 5-Methoxy-2-methylindole-3-ethanol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of esters from indolealkanols and amides from indolealkylamines as selective inhibitors of cyclooxygenase 2 and analgesic, antiinflammatory, and antipyretic agents)

RN 26766-01-8 CAPLUS

CN 1H-Indole-3-ethanol, 5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



103

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:234028 CAPLUS
DOCUMENT NUMBER: 118:234028
TITLE: Towards controllable molecular shuttles. 2
AUTHOR(S): Ashton, Peter R.; Bissell, Richard A.; Gorski, Romuald; Philp, Douglas; Spencer, Neil; Stoddart, J. Fraser; Tolley, Malcolm S.
CORPORATE SOURCE: Sch. Chem., Univ. Birmingham, Edgbaston/Birmingham, B15 2TT, UK
SOURCE: Synlett (1992), (11), 919-22
CODEN: SYNLES; ISSN: 0936-5214
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 118:234028
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The design and synthesis of a mol. shuttle I, in which the two components are a cyclobis(paraquat-p-phenylene)tetracationic macrocycle and a linear polyether chain intercepted by a 2,3,5-trisubstituted indole unit and a hydroquinol residue, and terminated by two 4-tritylphenyl ether functions, are described. The starting materials for this synthesis were 4-PhCH2OC6H4XH (X = NH, O), 4-Ph3CC6H4OH, and ClCH2CH2OCH2CH2OCH2CH2OH. A key step in the preparation of I is the Fischer indole synthesis of the linear component of the mol. shuttle from 4-Ph3C6H4OCH2CH2OCH2CH2OCH2CH2OC6H4NHNH and CO2CMe3-4 and ketal II.

IT 147553-59-1P
RL: PRP (Properties); PREP (Preparation)
(formation and spectra of, mol. shuttle synthesis in relation to)

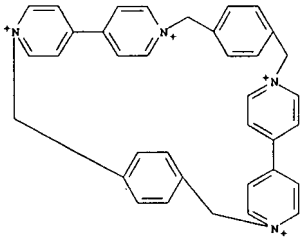
RN 147553-59-1 CAPLUS

CN 5,12,19,26-Tetraazoniaheptacyclo[24.2.2.22,5.27,10.212,15.216,19.221,24]tetraconta-2,4,7,9,12,14,16,18,21,23,26,28,29,31,33,35,37,39-octadecaene, tetrakis[hexafluorophosphate(1-)], compd. with 5-methoxy-2-methyl-1H-indole-3-ethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

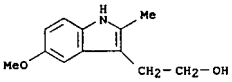
CRN 117271-76-8
CMF C36 H32 N4

L35 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



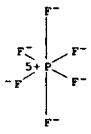
CM 2

CRN 26766-01-8
CMF C12 H15 N O2



CM 3

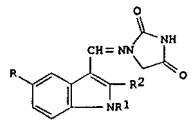
CRN 16919-18-9
CMF F6 P
CCI CCS



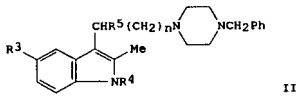
L35 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L35 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1988:630949 CAPLUS
DOCUMENT NUMBER: 109:230949
TITLE: 1H-Indole derivatives as calcium antagonists
AUTHOR(S): Garuti, Laura; Giovanninetti, Giuseppe; Bova, Sergio; Chiarini, Alberto
CORPORATE SOURCE: Dep. Pharm. Sci., Univ. Bologna, Bologna, I-40126, Italy
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1988), 321(7), 377-83
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:230949
GI



I



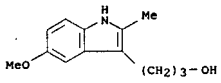
II

AB The preparation Ca antagonist and neg. inotropic activity of hydantoiniminomethylindoles, e.g., I (R = NO2, MeO; R1 = H, Bz, PhCH2, Et; R2 = Me, Cl, CO2Et) and benzylpiperazinoalkylindoles, e.g., II (R3 = NO2, MeO, Cl; R4 = H, Bz, PhCH2, CH2CH2NMe2, Et; R5 = H, Et; n = 0, 1, 2) are reported. Thus, condensation of 1-aminohydantoin.HCl with 2-methyl-5-nitroindole-3-carboxaldehyde gave 90% I (R = NO2, R1 = H, R2 = Me). Evaluations of Ca antagonist activity by inhibition of K+ induced contraction in rabbit auricolar artery strips and guinea pig taenia caeci found I (R = NO2 R1 = H, R2 = Me) was the most potent with an inhibiting concns. of 3 + 10-7. Most of the compds. evaluated showed neg. inotropic effects, the most active compound was I (R = MeO, R1 = H, R2 = Me).

IT 117752-70-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination-amination of, with benzylpiperazine)

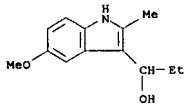
RN 117752-70-2 CAPLUS
CN 1H-Indole-3-propanol, 5-methoxy-2-methyl- (9CI) (CA INDEX NAME)

L35 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

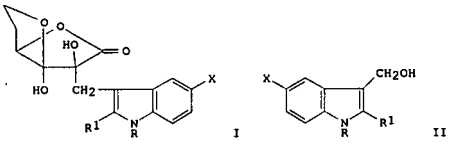


IT 117752-64-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and chlorination-amination of, with benzylpiperazine)

RN 117752-64-4 CAPLUS
CN 1H-Indole-3-methanol, α-ethyl-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



L35 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:520945 CAPLUS
DOCUMENT NUMBER: 107:120945
TITLE: Ascorbigen and its derivatives as depot-forms of ascorbic acid
AUTHOR(S): Bukin, Yu. V.; Plikhtyak, I. L.; Draudin-Krylenko, V. A.; Yartseva, I. V.; Orlova, L. M.; Preobrazhenskaya, M. N.
CORPORATE SOURCE: All-Union Cancer Res. Cent., Moscow, USSR
SOURCE: Bioorganicheskaya Khimiya (1987), 13(4), 539-45
CODEN: BIKHD7; ISSN: 0132-3423
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

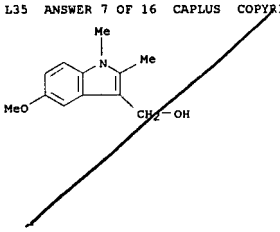


I

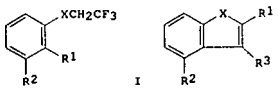
II

AB Ascorbigen derivs. (I, R = Me, Et or PhCH2; R1 = H or Me and X = H or OMe) were obtained by the reaction of 1-substituted-3-hydroxymethylindoles (II, R = Me, Et, or PhCH2; R1 = H or Me; X = H or OMe) with L-ascorbic acid in pH 4.0 citrate-phosphate buffer. The byproducts of the reaction were either dimerized or polymerized derivs. of II. In aqueous solns. at 37°, I dissociate to give L-ascorbic acid, the rate of decomposition being dependent on the substituents in I, and increasing with increasing pH and temperature I.p. injection of 1'-methylascorbigen to mice led to a steady increase in L-ascorbic acid levels in blood plasma. The kinetics of decomposition studies of 1'-methylascorbigen showed that the substituted ascorbigens might serve as the depot form of vitamin C, providing a prolonged-release effect.
IT 110345-10-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ascorbic acid)
RN 110345-10-3 CAPLUS
CN 1H-Indole-3-methanol, 5-methoxy-1,2-dimethyl- (9CI) (CA INDEX NAME)

L35 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



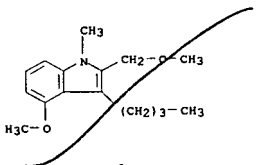
L35 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:101993 CAPLUS
DOCUMENT NUMBER: 106:101993
TITLE: Halocarbon chemistry. 3. Ortho metallation-induced cyclization of acetylenes: one-flask synthesis of 2,3-disubstituted benzofurans, thianaphthenes and indoles
AUTHOR(S): Johnson, Francis; Subramanian, Raghupathi
CORPORATE SOURCE: Dep. Chem., State Univ. New York, Stony Brook, NY, 11794, USA
SOURCE: Journal of Organic Chemistry (1986), 51(25), 5040-1
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:101993
GI



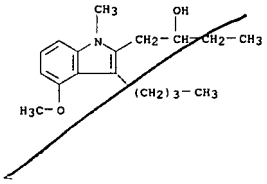
I

II

AB A new general organolithium-induced cyclization is described. Treatment of 2,2,2-trifluoroethyl Ph ethers I (X = O, R1 = R2 = H), the related thioethers I (X = S; R1 = Br, R2 = H), or the amines I (X = NMe; R1 = H, R2 = MeO) with four equivalent of an aryl or alkyl lithium reagent (R3Li) causes in almost all cases complete dehalogenation of the trifluoroethyl side chain with the concomitant introduction of an alkyl or aryl group (R3) at the acetylenic 2-position. This is followed apparently by ortholithiation to give the lithio intermediates and the latter then spontaneously cyclize to the 2-lithioheterocyles. Electrophilic quenching then leads to the corresponding heterocycles II [R1 = H, iodo, CH2OMe, CH2CH(OH)CH2Me; R2 = H, MeOR3 = Bu, Pr, MeCHEt, Ph] depending whether the electrophile is a proton or another electroneg. species.
IT 105230-41-9P 105230-42-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 105230-41-9 CAPLUS
CN 1H-Indole, 3-butyl-4-methoxy-2-(methoxymethyl)-1-methyl- (9CI) (CA INDEX NAME)

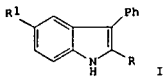


L35 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 105230-42-0 CAPLUS
CN 1H-Indole-2-ethanol, 3-butyl-α-ethyl-4-methoxy-1-methyl- (9CI) (CA INDEX NAME)



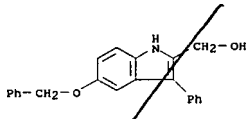
Karen Cheng

L35 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:405446 CAPLUS
DOCUMENT NUMBER: 85:5446
TITLE: A convenient synthesis of 3-phenyl-2-(2'-aminoethyl)indoles via 3-phenylindole-2-carboxaldehydes
AUTHOR(S): Gadaginamath, G. S.; Siddappa, S.
CORPORATE SOURCE: Dep. Chem., Karnatak Univ., Dharwar, India
SOURCE: Indian Journal of Chemistry (1975), 13(12), 1251-3
CODEN: IJOCAP; ISSN: 0019-5103
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

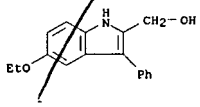


I

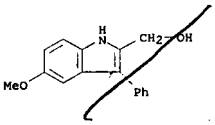
AB 5-Substituted 3-phenyl-2-(2'-aminoethyl)indoles I (R = CH2CH2NH2; R1 = Me, PhCH2O, EtO, MeO, H, Cl, Br) were prepared by condensation of I (R = CHO) with MeNO2 followed by reduction of I (R = CH:CHNO2). I (R = CH:CHNO2) exist mainly as inner nitronium salts.
IT 59394-34-2P 59394-35-3P 59394-36-4P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(prepare and oxidation of, indolecarboxaldehyde from)
RN 59394-34-2 CAPLUS
CN 1H-Indole-2-methanol, 3-phenyl-5-(phenylmethoxy)- (9CI) (CA INDEX NAME)



RN 59394-35-3 CAPLUS
CN 1H-Indole-2-methanol, 5-ethoxy-3-phenyl- (9CI) (CA INDEX NAME)



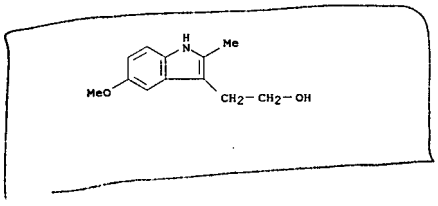
L35 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 59394-36-4 CAPLUS
CN 1H-Indole-2-methanol, 5-methoxy-3-phenyl- (9CI) (CA INDEX NAME)



L35 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:461810 CAPLUS
DOCUMENT NUMBER: 77:61810
TITLE: Hypotensive indoles
INVENTOR(S): Archibald, John Leleun
SOURCE: Brit., 9 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1273562		19720510	GB 1968-35230	19680724

GI For diagram(s), see printed CA Issue.
AB Pyridinioindole bromide (I, R = 4-acetamidopyridinio Br-, R1 = H), prepared from 3-(2-bromoethyl)-2-methylindole (I, R = Br, R1 = H) and 4-acetamidopyridine, was hydrogenated in 95% EtOH containing Et3N and Raney Ni for 4 hr at 400 psi and 75° to give I (R = 4-acetamidopiperidino, R1 = H) (II). Addnl. I (R = 4-acetamidopiperidino, R1 = MeO; R = 4-butyramidopiperidino, R1 = H) were prepared similarly.
II showed hypotensive activity in rats against autonomic amines.
IT 26766-01-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 26766-01-8 CAPLUS
CN 1H-Indole-3-ethanol, 5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



L35 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:125415 CAPLUS
DOCUMENT NUMBER: 74:125415
TITLE: Antiarrhythmic and β-blocking 3-methyl-4-(2-hydroxy-3-aminopropoxy) indoles
INVENTOR(S): Troxler, Franz
PATENT ASSIGNEE(S): Sandoz Ltd.
SOURCE: Ger. Offen., 36 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2038482	A	19710218	DE 1970-2038482	19700803
CH 514586	A	19711031	CH 1969-514586	19690805
CH 525884	A	19720731	CH 1970-525884	19700324
GB 1318050	A	19730523	GB 1970-35099	19700720
NL 7011029	A	19710127	NL 1970-11029	19700724
NL 7011028	A	19710209	NL 1970-11028	19700724
US 3696120	A	19721003	US 1970-58985	19700728
SE 369522	B	19740902	SE 1970-10622	19700803
SU 468414	A3	19750425	SU 1970-1473403	19700803
PL 81365	B1	19750830	PL 1970-142487	19700803
FR 2068461	A5	19710827	FR 1970-28683	19700804
FR 2068461	B1	19740111		
ES 382407	A1	19730416	ES 1970-382407	19700804
AT 313893	B	19740311	AT 1970-7098	19700804
JP 50022555	B	19750731	JP 1970-68283	19700804

PRIORITY APPLN. INFO.:

CH 1969-11918	A	19690805
CH 1969-15865	A	19691024
CH 1969-15866	A	19691024
CH 1970-4383	A	19700324
CH 1970-9536	A	19700624
GB 1969-37491	A	19690725
CH 1969-9536	A	19700624
CH 1970-9356	A	19700624

GI For diagram(s), see printed CA Issue.
AB The antiarrhythmic title compds. (I) with adrenergic β-receptor blocking activity were prepared by reaction of the 4-(2,3-epoxypropyl)indoles with amines, by debenzylation of the 4-(3-benzylaminopropoxy) derivs., by reduction of the 3-aminomethyl-4-[2-hydroxy-3-(benzylamino)propoxy]indoles (II) or the 2-carboxylates of II, or by reduction of the 4-(2-hydroxy-3-methyleneaminopropoxy)indoles. Thus, 4-benzyloxy-N,N-dimethylindole-2-carboxamide was reduced to 4-benzyloxy-2-dimethylaminoindole (III) with LiAlH4 in boiling THF. Quaternization of III with MeI and deamination with LiAlH4 in boiling dioxane gave 4-benzyloxy-2-methylindole, converted with HCHO and Me2NH in alc.-AcOH into 4-benzyloxy-2-methylgramine. This, quaternized with MeI

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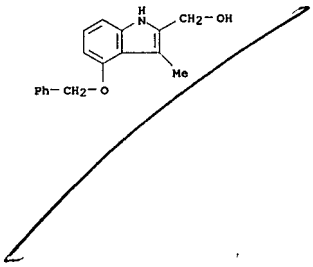
L35 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
and reduced with LiAlH4 in dioxane at 90° gave 2,3-dimethyl-4-benzyloxyindole, debenzylated (H-Pd/Al2O3) to 2,3-dimethyl-4-hydroxyindole (IV). NaOH (2.01 g) in 35 ml H2O was treated with 8.1 g IV in 35 ml dioxane, finally with 9.3 g epichlorohydrin in 25 ml 1:1 dioxane-H2O, under N, the mixt. stirred 24 hr at room temp., and the 2,3-dimethyl-4-(2,3-epoxypropoxy)indole boiled 15 hr with 30 ml iso-PrNH2 in 70 ml dioxane to give I (R = iso-Pr, R1 = Me). Among 7 compds. also prepd. were I (R and R1 given): pentyl, CO2Et; tert-Bu, CO2Et.

IT 31578-25-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 31578-25-3 CAPLUS

CN Indole-2-methanol, 4-(benzyloxy)-3-methyl- (8CI) (CA INDEX NAME)



L35 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1971:53406 CAPLUS
DOCUMENT NUMBER: 74:53406
TITLE: Synthesis of indole-2-carbaldehydes, 2-(2-aminoethyl)- and 2-(2-aminopropyl)indoles
AUTHOR(S): Siddappa, S.; Bhat, G. A.
CORPORATE SOURCE: Dep. Chem., Karnatak Univ., Dharwar, India
SOURCE: Journal of the Chemical Society [Section] C: Organic (1971), (1), 178-81
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English

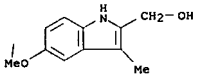
GI For diagram(s), see printed CA Issue.

AB Et indole-2-carboxylate derivs. (e.g. I) were reduced by LiAlH4 to indole-2-methanol derivs. (e.g. II). These were oxidized by MnO2 to indole-2-carboxaldehyde derivs. (e.g. III), which were also prepared from the indole-2-carboxylates by the McFadyen-Stevens reaction. The aldehydes reacted with MeNO2 and EtNO2, and the condensation products (e.g. IV and V) were reduced by LiAlH4 to 2-(2-aminoethyl)indoles (e.g. VI) and 2-(2-aminopropyl)indoles (e.g. VII), resp.

IT 30464-82-5P 30464-84-7P 30464-87-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

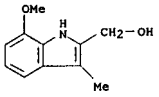
RN 30464-82-5 CAPLUS

CN Indole-2-methanol, 5-methoxy-3-methyl- (8CI) (CA INDEX NAME)



RN 30464-84-7 CAPLUS

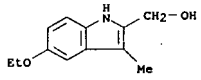
CN Indole-2-methanol, 7-methoxy-3-methyl- (8CI) (CA INDEX NAME)



RN 30464-87-0 CAPLUS

CN Indole-2-methanol, 5-ethoxy-3-methyl- (8CI) (CA INDEX NAME)

L35 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L35 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1970:466782 CAPLUS
DOCUMENT NUMBER: 73:66782
TITLE: Transformation of quinine into indole alkaloids. IV. Configuration of cinchonamine at C-8
AUTHOR(S): Sawa, Yoshiro K.; Matsumura, H.
CORPORATE SOURCE: Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, Japan
SOURCE: Tetrahedron (1970), 26(12), 2923-9
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Dihydrocinchonamine was synthesized from quinine, and the configuration at C-8, heretofore ambiguous, was clarified.

IT 28337-31-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

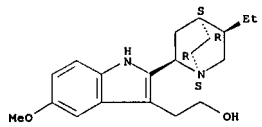
RN 28337-31-7 CAPLUS

CN Thiocyanic acid, compd. with [1S-(1α,2β,4α,5β)]-2-(5-ethyl-1-azabicyclo[2.2.2]oct-2-yl)-5-methoxy-1H-indole-3-ethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 28337-32-8
CMF C20 H28 N2 O2

Absolute stereochemistry.



CM 2

CRN 463-56-9
CMF C H N S

Karen Cheng

L35 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:121363 CAPLUS
DOCUMENT NUMBER: 72:121363
TITLE: Antiinflammatory 3-[2-[4-(substituted-benzamido)piperidino]ethyl]indoles
INVENTOR(S): Archibald, John L.; Jackson, John Lambert
PATENT ASSIGNEE(S): John Wyeth and Brother Ltd.
SOURCE: S. African, 38 pp.
CODEN: SFXXAB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 6803204		19691117	ZA	
DE 1770460			DE	
FR 1582086			FR	
FR 7787			FR	
GB 1218570			GB	
US 3527761		19700908	US	19680515
PRIORITY APPLN. INFO.:			GB	19670524
			GB	19680301

OTHER SOURCE(S): MARPAT 72:121363
AB Title compds. with antiinflammatory activity and (or) cardiovascular and (sometimes) control nervous system activity, were prepared Thus, BzCl was added dropwise to an ice-cooled solution of 4-aminopyridine in pyridine to yield 4-benzamidopyridine. This (1.98 g) and 3-(2-bromoethyl)indole (2.24g) in 15 ml absolute EtOH was refluxed 2 hr, to yield 4-benzamido-1-[2-(3-indolyl)ethyl]pyridinium bromide (I) as the hydrate, m. 267-9° (EtOH-H2O). NaBH4 (6.0g) was added over 30 min to a stirred suspension of 2.0 g I in 100 ml MeOH and the mixture stirred 1 hr to give 1.54 g 3-[2-(4-benzamido-1,2,5,6-tetrahydro-1-pyridyl)ethyl]indole, m. 209-11° (MeOH). Similarly prepared were the following 3-[2-(R-substituted)-ethyl]indoles (R and m.p. given): 3-benzamido-1,2,5,6-tetrahydro-1-pyridyl, 180-2° (MeCN); 4-benzyloxycarbonylamino-1,2,5,6-tetrahydro-1-pyridyl, 162-4° (EtOH); 4-[4-chlorobenzamido]-1,2,5,6-tetrahydro-1-pyridyl, 229-30° (EtOH-Me2SO); 4-[2,2-diphenylacetamido]-1,2,5,6-tetrahydro-1-pyridyl, 197-8° (EtOH); 4-benzylamino-1-pyridyl, 132-4° (C6H6-80-100° petroleum ether); 4-benzamido-1-piperidyl, 208-10° (EtOH); and 3-benzamido-1-pyridyl, 135-40° (aqueous EtOH). Also prepared were the following 3-[2-[4-(R-substituted)-1-piperidyl)ethyl]indole. (R and m.p. given): 4-chlorobenzamido, 230-2° (EtOH); 4-methoxybenzamido, (as the HCl salt hydrate), 284-6° (EtOH-H2O); acetamido, 167-8° (EtOAc); amino, 106-10° (aqueous MeCN); 3-methoxybenzamido, 149-50° (MeCN); 2-methoxybenzamido, 152-4°; 3,4,5-trimethoxybenzamido(hydrate), 105-8° (EtOHH2O); indole-3-carboxamido, 242-4° (aqueous Me2CO); 2,2-diphenylacetamido, 160-2° (ag. EtOH); 2-methylbenzamido,

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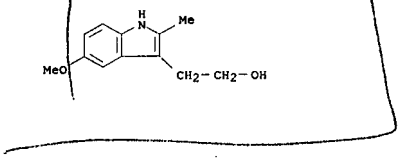
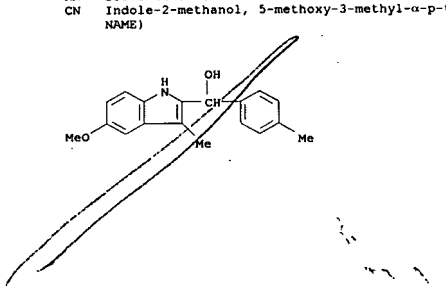
186-9°; 3-methylbenzamido, 172-4°; 4-methylbenzamido, 200-2°; 2-furancarboxamido, 146-8°; 2-chlorobenzamido, 163-4°; 3,4-methylenedioxybenzamido, 189-90°; 2-carboxybenzamido(hydrate), 165-70° (EtOH-H2O); 3-trifluoromethylbenzamido, 186-8°; 4-phenylbenzamido(monohydrate), 271-2°; and 4-phenylacetamido, 165-8°. Also prepd. were the following 3-[2-(R-substituted-ethyl]-2-methylindoles (R and m.p. given): 4-benzamido-1-piperidyl, 209-11° (aq. EtOH); 4-[4-methoxybenzyamido]-1-piperidyl(monohydrate), 110-14° (EtOH); and 4-(4-chlorobenzamido)-1-piperidyl (HCl salt), 243-5° (EtOHEt2O). Also prepd. were the following 3-(R-substituted)-1-methylindoles. (R and m.p. given): 2-(4-benzamido-1-piperidyl)-ethyl, 178-9° (ag. EtOH); 2-[4-(4-chlorobenzamido)-1-piperidyl] ethyl, 212-14°; 2-[4-(-methylbenzamido)-1-peperidyl]ethyl, 198-9°; and 2-[4-(4-methoxybenzamido)-1-piperidyl]ethyl, 198-9°. Also prepd. were the following 3-(R-substituted)-1-benzylindoles. (R and m.p. given): 2-(4-benzamido-1-piperidyl)ethyl, 152-3° (aq. EtOH); 2-[4-(4-chlorobenzamido)-1-piperidyl]ethyl, 193-4°; and 2-[4-(4-methoxybenzamido)-1-piperidyl]ethyl, 191-2°. Also prepd. were the following 3-[2-(R-substituted)-1-oxoethyl]indoles (R and m.p. given): 4-benzamido-1-piperidyl, 204-6°; 4-(4-chlorobenzamido)-1-piperidyl, 231-3°; and 4-(4-methoxybenzamido)-1-piperidyl, 227-9°; also prepd. were: 3-[2-(4-benzamido-1-piperidyl)ethyl]-5-methoxy-2-methylindole, m. 180-1° (EtOAc); and 3-[3-(4-benzamido-1-piperidyl)propyl]indole, m. 179-80° (aq. EtOH).
IT 26766-01-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 26766-01-8 CAPLUS
CN 1H-Indole-3-ethanol, 5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



L35 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1969:512729 CAPLUS
DOCUMENT NUMBER: 71:112729
TITLE: Synthesis of aryl-2-indolylcarbinol derivatives
AUTHOR(S): Shvedov, V. I.; Alekseev, V. V.; Grinev, A. N.
CORPORATE SOURCE: Vses. Nauch.-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1969), 3(6), 8-10
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB The title compds. usually display a spectrum of biol. activities. Derivs. were prepared by reduction of 0.1 mole 2-aryl-3-methylindole in 500 ml. EtOH with 100 g. Zn and 80 g. NaOH. The reaction mixture was refluxed 10 hrs. with stirring, separated from the residue, and poured into water with ice. The precipitated I were prepared (R, R', R", % yield, and m.p. given): H, H, Me, 94, 131-1.5°; H, Me, H, 98.5, 146-7°; Me, Me, H, 93.2, 87-7.5°; H, Me, Me, 94.3, 118-19°; H, Me, MeO, 93.8, 121-2°; H, MeO, Me, 90, 130-1°. The structure of I was determined by ir absorption spectra. Derivs. of I with unsubstituted N are hygroscopic and light-sensitive.
IT 23876-44-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23876-44-0 CAPLUS
CN Indole-2-methanol, 5-methoxy-3-methyl-α-p-tolyl- (8CI) (CA INDEX NAME)



L35 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:403932 CAPLUS
DOCUMENT NUMBER: 65:3932
ORIGINAL REFERENCE NO.: 65:691b-e
TITLE: Antiinflammatory indole derivatives
PATENT ASSIGNEE(S): Merck & Co., Inc.
SOURCE: 105 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6508553		19660103	NL 1965-8553	19650702
PRIORITY APPLN. INFO.:			US	19640702

GI For diagram(s), see printed CA Issue.
AB I (R1 = COC6H4Cl-4) (II) were prepared To a solution of 0.02 mole I (R = R1 = H) (III), 0.22 mole HNMe2, and a trace of HCl in 250 ml. EtOH was added 0.22 mole 40% H2CO and the whole refluxed 5 hrs. to give I (R = CH2NMe2, R1 = H). A solution of 0.021 mole III in 20 ml. HCONMe2 was added to a cold suspension of 52% NaH in mineral oil and 250 ml. HCONMe2, the mixture stirred 20 min., cooled, and treated with 0.0222 mole 4-ClC6H4COCl, and the mixture stirred 16 hrs. to give II (R = H). The following I (R1 = H) were prepared (R given): CHO; CH:NEt; Ac; CH2NHEt; CH2N:CHPh; CH2NEt2; CH:CMeNO2; CH2CHMeNH2; CH2CHMeNHEt; CHMeCOCl (IV); 1-methyl-butanon-1-yl (from IV and Et2Cd); CHMeCHEt:NEt; CHMeCHMeOH; CHMeCHEtBr; CHMeCHEtCN; CHMeCHEtNH2.HCl; CHMeCHEtN:CHPh; CHMeCHEtNHEt; CHMeCHEtCHO; CHMeCHEtCH:NEt; CHMeCHEt:CHNO2. The following II were prepared (R given): CH:NEt; CH:CHCMeNO2; CHMeCHEt:NEt; CHMeCHEtCN; CHMeCHEtCH:NEt; CH2N:CHPh; CH2-NH2.HCl; CH2NMe2; CH2NH2; CH2NEt2; CH2CHMeNH2; CHMeCHEtNH2; CHMeCHEtNHEt; CHMeCHEtCH2NH2; CHMeCHEtCH2NHEt; CHMeCHEtCH2NH2.HCl; CHMeCHEtN: CHPh; CHMeCHEtNH2.HCl; CHMeCHEtCH2NHEt.HCl; CHMeCHEtCH2NEt2; CH2CONH2 (m. 219-21°); CH2CN; CH2CH2NH2.HCl; CH2CH2NEt2; CH2CH2NMe2 (from I (R = CH2CH2NMe2, R1 = H), NaH, and 4-O2NC6H4OCOC6H4Cl-4 (m. 137°) in HCONMe2). Also prepared was: 1-p-fluorobenzoyl-3-(β-morpholinoethyl)-5-hydroxyindole hydrochloride.
IT 6264-12-6P, Indole-3-ethanol, 5-methoxy-α,β,2-trimethyl-
RL: PREP (Preparation)
(preparation of)
RN 6264-12-6 CAPLUS
CN Indole-3-ethanol, 5-methoxy-α,β,2-trimethyl- (7CI, 8CI) (CA INDEX NAME)